Predictive Engineering Tools for Injection **Molded Long Carbon Fiber Thermoplastic**

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LM115

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Overview:

<u>Timeline</u>

- Project Start 2014
- Final Report Issued December 2016

Budget

- Barriers addressed
- Computational Modeling
- Predictive Engineering
- Composite Manufacturing
- \$847,820 in FY 2013/14 from VTO (41% of total project cost)
 - \$1,198,000 cost share from Partners (59% of total project Cost)

Partners and Collaborators

ORNL: National Laboratory

FORD: OEM

BASF: Material Supplier

PlastiComp: Tier I supplier

Moldex 3D: Predictive Modeling

Univ. of Illinois: University

Virginia Tech: University

Project Objective and Team

Objective:

Implement and validate computational tools for prediction of fiber orientation and fiber length distribution in injection molded long carbon fiber thermoplastic composites for automotive applications to meet goals in the DOE-VT MYPP.

Relevance: Given an input fiber length in the injection process, (1) can we predict the fiber orientation, distribution and orientation at any given location and thus the properties? If so, could we then (2) can we start with desired properties at a given location and predictively engineer (through computational methods) the system to give us that?

Team:

ORNL: Fiber orientation and fiber length distribution measurement

FORD: Part selection and previous results, Moldflow analysis

BASF: Materials and tools available for the project

PlastiComp: Pellet manufacturing and molding resources

Moldex 3D: Injection molding simulation

University of Illinois: Fiber breakage model

Virginia Tech: Rheology and FOD measurements

Resources

Participant	Organization Type		Cost Share*	Total Budget*	Cost Share % of Total Project
ORNL	DOE/NNSA National Laboratory/FFRDC	\$500.12	\$0	\$500.12	0%
Ford Motor Company	For Profit Company	\$100	\$300	\$400	15%
Moldex3D North America	For Profit Company	\$0	\$600	\$600	31%
BASF	For Profit Company	\$0	\$200	\$200	10%
PlastiComp Inc.	For Profit Company	\$0	\$80	\$80	4%
Virginia Polytechnic Institute and State University	nd Institution of Higher Education		\$17.72	\$117.72	1%
University of Illinois	Institution of Higher Education	\$47.7	\$0	\$47.7	0%
Total		\$747.82	\$1,198	\$1,946	62%

Timeline:

Project Start: April 24 2013

Project End: December 31 2016

Milestones and Tasks

Task 1 - Project Management and Planning

Phase 1. Model Integration

Task 2 – Selection of representative 3-D prototype part ✓



Go/No Go Decision Point: ORNL shall not proceed with Tasks 1 through 9 prior to written approval of the 3-D part by the DOE. Written approval may be in electronic form.



Task 3 - Simulation of Plaque geometry with Moldex3D and Moldflow software



Task 4. Implementation of reduced order Phelps-Tucker fiber breakage model in 🜙 Moldex3D



Task 5. Prediction of fiber orientation and FLD for CF complex 3-D part



Phase 2. Validation of Composite Fiber Length and Geometric **Distribution**

Task 6. Fiber orientation and FLD in CF 3-D complex part measurement



Task 7. Molding of complex 3-D part \checkmark



Go/No Go Decision Point: ORNL shall not proceed with Tasks 7.1 through 9 prior to written approval of the molding resources by the DOE. Written approval may be in electronic form.

Task 8. Comparison of experimental data to predictions from Phase 1 🗸



Task 9. Weight saving and cost estimate analysis



Approach to Address State of the Art and Barriers

Target: Validate CF **length** to 15% of model prediction on **flat plaques** using the reduced-order fiber breakage model.

Target: Validate CF **length** to 15% of prediction for the **complex part** using the reduced-order fiber breakage model.

Target: Validate CF **orientation** to 15% of prediction for **complex part** using the fiber orientation model.

Gap: A reduced-order fiber breakage model is not available in a commercial code. A reduced-order model is not validated for injection-molded CF-reinforced thermoplastics.

Gap: Fiber orientation and length models are not validated in commercial codes for injection-molded CF-reinforced thermoplastics.

Gap: An experimental dataset for validation of fiber orientation and fiber length models, specifically for CF, is not available for parts with complex geometries.

Technical Accomplishments and Progress - Samples and Materials



Edge gated plaque

 Three samples along flow length are selected for FLD and FOD analysis in plaques

Materials and molding conditions

	Fiber	Back	Fill
Polymer	Loading [%]	Pressure	Speed
Polyamide	40%	Low	Slow
Polyamide	40%	High	Fast
Polyamide	20%	Low	Slow
Polypropylene	40%	Low	Slow
Polypropylene	40%	High	Fast
Polypropylene	20%	Low	Slow







Front, back and side of seatback part

- Seat-back contains many complex geometry features
- Details of this part were optimized to maximize fiber length

Technical Accomplishments and Progress - Molding Trials

Plaques and seatback parts were molded on different machines to accommodate part size and material residence time.





PlastiComp 350 ton press with plaque tool





ASPN 850 ton press with seatback tool

- Purge trials were performed prior to molding trials to compare fiber lengths from the machines
- Screw for ASPN machine was modified to increase fiber length for seatback parts
- Screw modification resulted in longer fiber lengths

Purge trials fiber length for PA6,6/40% CF (initial fiber length was 10mm)

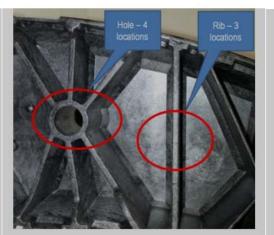
	Specimen description	Fibers	Ln (mm)	Lw (mm)
1	Plasti Comp	2185	4.06	7.33
2	ASPN old screw	2134	1.69	4.44
4	ASPN new screw	2065	2.58	5.06





Technical Accomplishments and Progress - Feature Based Analysis







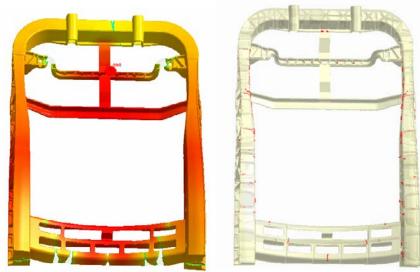




Sample Locations were chosen to include the most complex fiber flow direction changes:

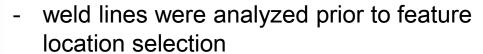
- > Ribs
- > Holes
- Change in flow direction
- Thickness Variations

Technical Accomplishments and Progress - Feature Based Analysis

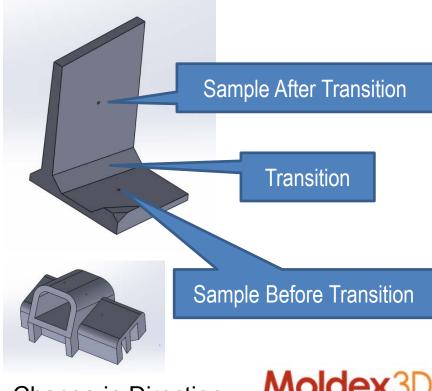


Weld lines from simulation

Features analyzed:



FOD and FLD is analyzed before and after transition









Hole



Flat Section

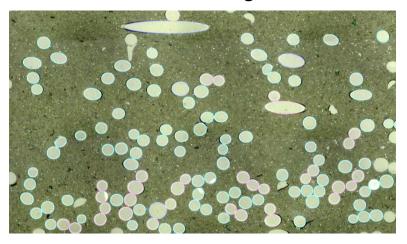




Gate

Measurement Technique Modification

Automation of un-ambiguous fiber orientation

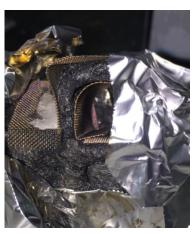


- Each ellipsoidal filament cross-section results in two possible fiber orientations
- Ambiguity is not acceptable for nonsymmetric samples
- Automated technique for un-ambiguous fiber orientation measurement was developed at ORNL

Fiber Sample Isolation for FLD measurements



Molded Sample



Pyrolyzed Sample



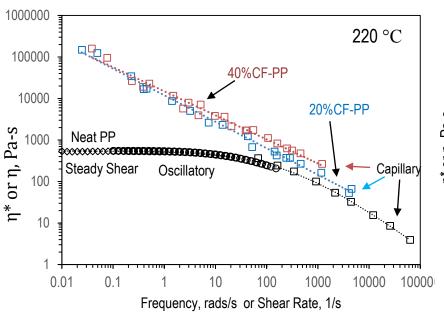
Isolated Fibers

- Partially constrained pyrolysis is necessary for fiber sample isolation
- Multiple fiber samples are selected from a single pyrolyzed sample

Bulk Viscosity Data



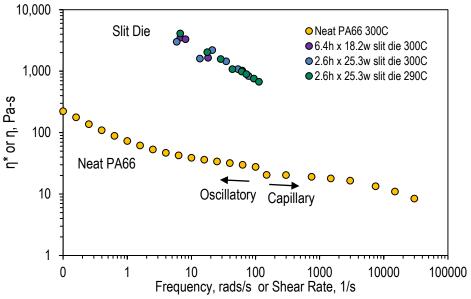
Carbon Fiber - Polypropylene



$$L_n = 0.84 mm$$
$$L_w = 1.9 mm$$

More breakage in capillary rheometry experiments due to sample preparation

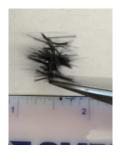
40% Carbon Fiber – Polyamide 6,6



$$L_n = 1.4 mm$$

$$L_w = 3.4 mm$$

Some bundles were observed in the slit die extrudate



Plaque measurements

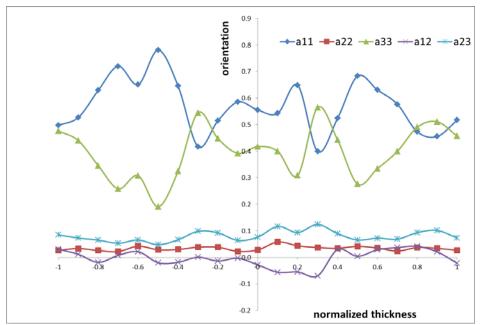
PA6,6/40% CF, slow fill speed, low back pressure

Fiber domains and voids present in the sample

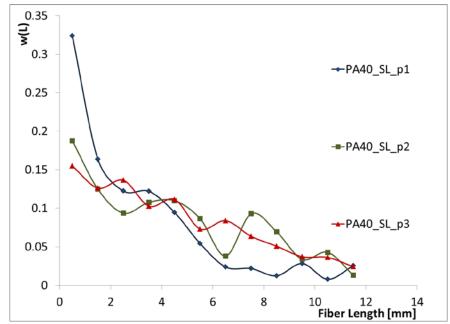


Fiber length average

Sample	Lw [mm]
PA40SL_p1	2.89
PA40SL_p2	4.30
PA40SL_p3	4.31

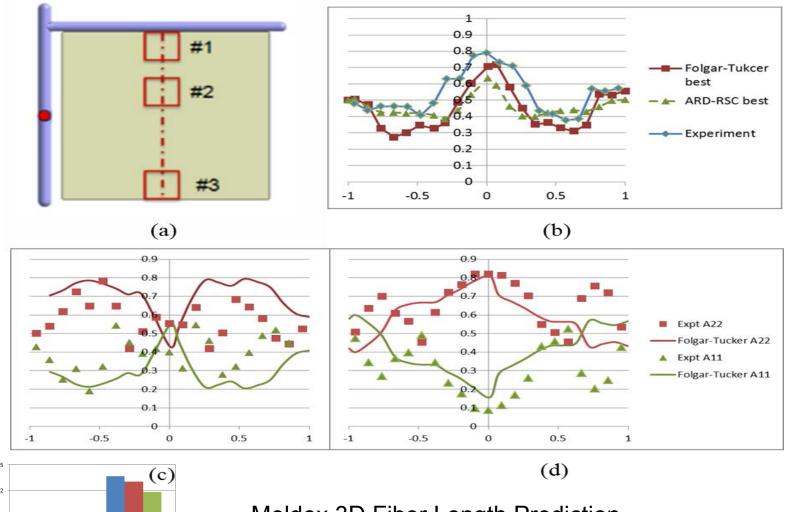


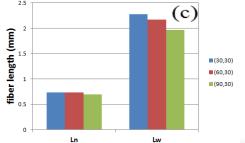
FOD for PA40SL – mid plaque position



FLD for PA40SL

Plaque Fiber Orientation and Length





Moldex 3D Fiber Length Prediction includes an empirical model for screw.



Plaques - Fiber Orientation and Length LM115 Comparison

Averaged value of flow directional fiber orientation component A₁₁ of ORNL experimental data and Moldex3D prediction showing accuracy of prediction.

Location	Averaged A ₁₁ (ORNL experiment)	Averaged A ₁₁ (Moldex3D prediction)	Accuracy of Prediction (%)
1	0.424	0.421	0.6
2	0.571	0.574	0.7
3	0.304	0.302	0.6

Averaged value of cross-flow directional fiber orientation component A₂₂ of ORNL experimental data and Moldex3D prediction showing accuracy of prediction.

Location	Averaged A ₂₂ (ORNL experiment)	Averaged A ₂₂ (Moldex3D prediction)	Accuracy of Prediction (%)
1	0.542	0.556	2.8
2	0.396	0.415	4.8
3	0.653	0.682	4.5

Number-averaged fiber length (Ln) of flow directional component of ORNL experimental data and Moldex3D prediction showing accuracy of prediction.

Location	Ln (ORNL experiment)	Ln (Moldex3D prediction)	Accuracy of Prediction (%)
1	0.633	0.668	2.2
2	0.799	0.628	21.4
3	0.993	0.636	36.0

Weight-averaged fiber length (Lw) of flow directional component of ORNL experimental data and Moldex3D prediction showing accuracy of prediction.

Location	Lw	Lw	Accuracy of Prediction
	(ORNL experiment)	(Moldex3D prediction)	(%)
1	2.894	2.730	5.7
2	4.296	2.460	42.7
3	4.305	2.536	41.1

Plaques - Stiffness Prediction Comparison

Calculated stiffness from measured and predicted fiber orientation showing accuracy of prediction.

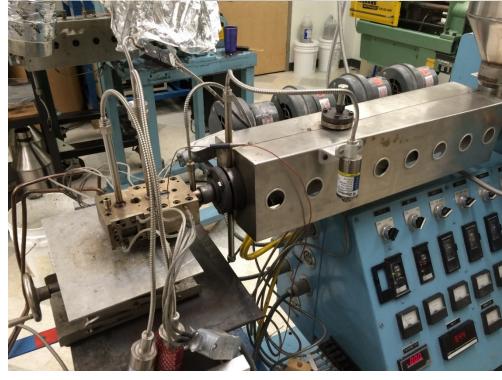
Tensile Modulus							
Location	E11 [Pa] (predicted orientation)	E11 [Pa] (measured orientation)	Accuracy of Prediction (%)				
1	1.58E+10	1.57E+10	1.17E+00				
2 (average)	1.44E+10	1.45E+10	7.39E-01				
3	1.05E+10	1.58E+10	4.02E+01				
	E22 [Pa] (predicted orientation)	E22 [Pa] (measured orientation)	Accuracy of Prediction (%)				
1	1.91E+10	2.06E+10	6.43E+00				
2 (average)	2.10E+10	2.06E+10	1.77E+00				
3	2.44E+10	2.06E+10	1.72E+01				
	Flexural	Modulus					
Location	D11 [Pa m³] (predicted orientation)	D11 [Pa m³] (measured orientation)	Accuracy of Prediction (%)				
1	4.25E+01	4.96E+01	1.56E+01				
2 (average)	4.33E+01	4.40E+01	1.73E+00				
3	6.29E+01	5.02E+01	2.26E+01				
	D22 [Pa m³] (predicted orientation)	D22 [Pa m³] (measured orientation)	Accuracy of Prediction (%)				
1	5.50E+01	5.04E+01	8.85E+00				
2 (average)	5.52E+01	5.70E+01	3.19E+00				
3	3.49E+01	5.09E+01	3.73E+01				

Bulk Rheology Measurements

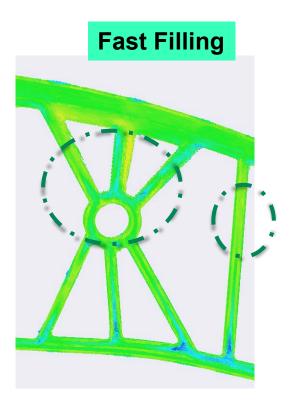
- Little literature information on the rheology of (long) carbon fiber composites
- Objective: produce bulk viscosity data of long fibers for use in molding simulations
- Capillary rheometry for CFpolypropylene composites
- CF-PA66 composite bulk data was unreliable in capillary rheometer
- A slit die rheometer was used with a single screw extruder to capture the bulk 40%CF-PA66 viscosity





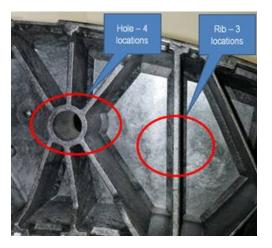


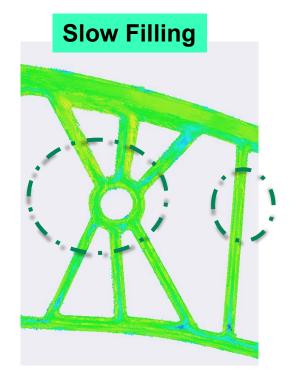
Seatback Fiber Orientation and Length LM115

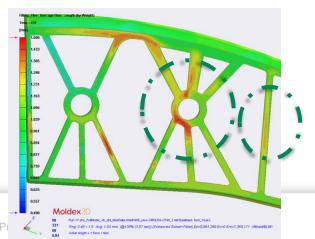


Fast > Slow

Fiber Orientation

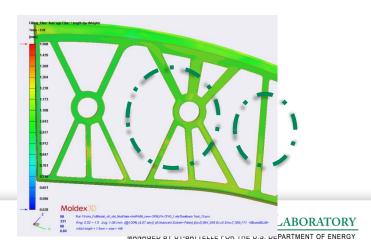




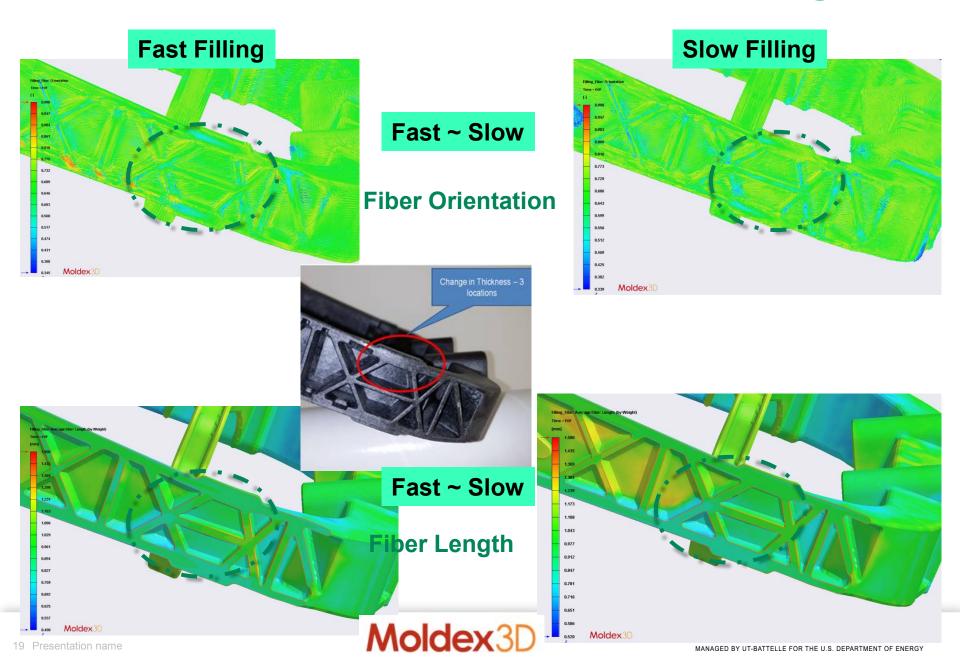


Fast > Slow
Fiber Length





Seatback Fiber Orientation and Length LM115



Model-Experiment Comparison for Complex Part

Model – experiment comparison of first eigenvalue of second order orientation tensor for polyamide with 40% CF molded with low back pressure and slow fill speed.

Location	Moldflow	Moldex3D	Experiment	Moldflow Prediction Deviation (%)	Moldex3D Prediction Deviation (%)
Direction Change 1	0.82	0.57	0.75	8.9	24.2
Direction Change 2	0.72	0.55	0.62	16.4	11.1
Direction Change 3	0.58	0.62	0.63	8.0	2.5
Thickness 1	0.96	0.76	0.72	32.7	5.1
Thickness 2	0.96	0.75	0.69	39.8	9.2
Rib	0.98	0.71	0.77	27.4	8.2
Flat Mutual Point	0.95	0.71	0.67	41.2	5.5
Hole 1	0.90	0.70	0.79	13.7	11.2
Hole 2	0.89	0.70	0.78	13.1	10.2

Cost Analysis

Cost and Mass Analysis was performed using the seatback and then also to a prototype oil pan system that Ford had.

Seatback Cost	Mass (kg)	Cost Penalty	Oil Pan Cost	Mass (kg)	Cost Penalty
Cast Al	3.56		Cast Al	3.0	
PA66-40% SCF	1.75		PA66 40% LCF	1.6	
Mass saved	1.81 (50%)		Mass Saved	1.4 (48%)	
Cost penalty (\$/part)		\$6.29	Cost Penalty (\$/Part)		\$6.02
Cost penalty (\$/kg saved)		\$3.48	Cost Penalty (\$/kg saved)		\$4.30

	Oil Pan		Seat Back	
	SI Units	English Units	SI Units	English Units
Number of parts per vehicle	1	1	4	4
Mass saved per part	1.4 kg	3.08 lb	1.81 kg	3.98 lb
Cost penalty per part	\$6.02	\$6.02	\$6.29	\$6.29
Total mass saved per vehicle	1.42 kg	3.08 lb	7.24 kg	15.92 lb
Cost penalty per vehicle	\$6.02	\$6.02	\$25.16	\$25.16
Total vehicle cost penalty per unit mass	\$4.30/kg	\$1.95/lb	\$3.48/kg	\$1.58/lb

Remaining Challenges, Barriers, and Future Research

This project completed in December 2016 and no further efforts are planned.

Remaining Challenges (to assist industry):

- Further refinement of the models would help industry.
- Development of and interfacing of fiber length attrition models for various screw designs would be of great benefit.
- Integration with models upstream and downstream of this part of the process would be of benefit to industry.

Summary

Integrated industry—university— national laboratory team has addressed technology gaps in the area of long fiber reinforced thermoplastic injection molding:

- Reduced order breakage model was implemented in a commercially available software
- Parts with complex geometry have been molded under controlled conditions
- Fiber length has been maximized with currently available technology
- Experimental procedures have been modified to allow evaluation of FLD and FOD in complex parts
- Flow simulation within a complex part has been performed with two leading software packages Moldex 3D and Moldflow
- FLD and FOD measurements were performed in complex part
- Blind comparison of experimental and predicted results was performed
- Cost analysis was performed for long carbon fiber injection molded part

Discussion

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